2016

Predictive Formula for Electron Penetration Depth of Diverse Materials over Large Energy Ranges

Anne C. Starley
Utah State University

Gregory Wilson
Utah State University

Lisa D. Montierth
Utah State University

JR Dennison
Utah State Univesity

PREDICTIVE FORMULA FOR ELECTRON PENETRATION DEPTH OF DIVERSE MATERIALS OVER LARGE ENERGY RANGES

Anne Starley, Gregory Wilson, Lisa Phillipps and JR Dennison

Utah State University Dept. of Physics, 4415 Old Main Hill, Logan, UT 84322-4415 USA, anne.starley@aggiemail.usu.edu

ABSTRACT

An empirical model that predicts the approximate electron penetration depth—or range—of some common materials has been extended to predict the range for a broad assortment of other materials. The electron range of a material is the maximum distance electrons can travel through a material, before losing all of their incident kinetic energy. The original model used the Continuous Slow Down Approximation (CSDA) for energy deposition in a material to develop a composite analytical formula which estimated the range from <10 eV to >10 MeV with an uncertainty of <20% using a single empirical fitting parameter, N_V^{eff}, which is termed the effective number of valence electrons. N_V^{eff} was empirically calculated for >200 materials which have tabulated range and inelastic mean free path data in the NIST ESTAR and IMFP databases. Correlations of N_V^{eff} with key material constants (*e.g.*, density, atomic number, atomic weight, and band gap) were established for this large set of materials. Somewhat different correlations were found for different sub-classes of materials (*e.g.*, solids/liquids/gases, conductors/semi-conductors/insulators, elements/compounds/polymers/ composites). A predictive formula was developed to accurately determine N_V^{eff} for arbitrary materials.

1. INTRODUCTION

The range or penetration depth, *R*, describes the maximum distance electrons can travel through a material, given an initial incident energy, before they lose all of their kinetic energy and come to a rest. It is a common way to parameterize electron interactions with materials.[1,2]

An approximate range expression was developed by merging well known semi-empirical models for the interaction of electrons with materials in different energy regimes by employing the continuous slow down approximation (CSDA); details are provided in [3]. Using the CSDA, a continuous, simple, composite, analytic formula—with the single empirical free parameter, N_V^{eff}— approximates the range (10^{-9} m to 10^{-2} m) over an extended energy span (<10 eV to >10 MeV). Agreement with available databases of electron interactions are within <20% for many conducting, semiconducting, and insulating materials.[4]

This work was supported by a Utah State University Undergraduate Research and Creative Opportunities Grant and funding through NASA GSFC and the James Webb Space Telescope.

This paper describes efforts to develop a predictive formula for this single fitting parameter based solely on the stoichiometry of the material and its basic material properties. The validity of this process is examined by comparison of the range predicted with this formula to tabulated range data in the NIST databases.[1,2]

2. RANGE ACCURACY OF PREDICTED N_V^{eff}

Range values as a function of energy were determined as empirical N_V^{eff} values derived from fits to the NIST database range and inelastic mean free path values. Original fits to ~20 materials[3] have now been extended to almost all of the >200 diverse materials found in the NIST databases.[1,2] These were found to give good fits with differences typically less (often much less) than ±20% over full 10 eV<*E*<10 MeV spans.[3]

3. PREDICTIVE FORMULA FOR N_V^{eff}

A simple formula was found to predict the single range parameter, N_V^{eff}:

$$N_V^{pre}(Z_m) = N_o \, {Z_m}^{n_0} + N_{offset} \, . \qquad (1)$$

This formula was found through extensive analysis of much more complex predictive formula for N_V^{eff} involving products of power law terms for density, mean atomic number and weight, and bandgap plus other properties including plasmon energy, conductivity, phase, and more.[5] This general fit for N_V^{eff} was evaluated using general least squares fit analysis methods to simultaneously determine the best estimates for fitting parameters for each material property.

Remarkably, this predictive formula for effective number of valence electrons was a function of only mean atomic number, Z_m, which can be easily determined from the stoichiometric formula for compounds or from elemental fraction for composite materials.

4. RANGE ACCURACY OF PREDICTED N_V^{eff}

Range values as a function of energy predicted with empirical N_V^{eff} values derived from fits to the NIST database range and inelastic mean free path values were found to give good fits with differences typically less (often much less) than ±20% over full 10 eV<*E*<10 MeV spans.[3] Fig. 1(a) shows the range of Sr calculated using both empirical N_V^{eff} and predicted N_V^{pre} values; Sr and Au are two of the materials with the worst agreement with measured data in the NIST databases.

Table 1. Constants and goodness of fit for predictive N_V^{pre} model.

Materials	N_o	n_o	N_{offset}	χ^2_{Nv}	R
All	21.223	0.112	22.854	0.0061	0.987
Insulators	22.712	0.101	24.114	0.0042	0.987
Conductors	24.219	0.107	26.690	0.0052	0.949
Semiconductors	14.817	0.153	16.585	0.0005	0.990

To better gauge the validity of the predictive formula for N_V^{pre} as given by Eq. (1), comparisons of the range were made using the empirical N_V^{eff} and predicted N_V^{pre} values with excellent results. By plotting this prediction, N_V^{pre}, versus the best values of N_V^{eff} from direct fits to the NIST database, goodness of fit metrics χ^2_{Nv} and R allows quantification of the quality of the fits. The fitting parameters were then used to calculate N_V^{pre} using Eq. (1). Table 1 show the results of these comparisons, for all materials from the NIST database, and subdivided by conduction type. Fig. 1(b) shows the percent differences between ranges calculated with empirical N_V^{eff} and predicted N_V^{pre} values for several representative materials.

5. CONCLUSIONS

Simulations were performed to test the sensitivity of N_V^{eff} and the range to materials parameters; these suggest that reasonably accurate results were achievable with modest precision of the parameters. These correlations have led to methods using only basic material properties to predict N_V^{eff} and the range for additional untested materials which have no supporting range data. These calculations are of great value for studies involving energetic electron bombardment, such as electron spectroscopy, spacecraft charging, or electron beam therapy. Efforts are underway to create a user tool available to the scientific community to estimate the range of an arbitrary material with modest accuracy over an extended span of incident electron energies.

Future work will:

- Create an online range prediction calculator that will be able to produce the range of a material with only input of the common material parameters.
- Develop a better relativistic approximation to improve range predictions above m_ec^2=0.5 MeV.
- Imrove N_V^{pre} predictions by adding additional Z_m dependence and orbital corrections in Eq. (1).
- Study the HOMO-LUMO gap, E_{LH}, as a possible surrogate for liquids and gases of the band gap in solids.
- Model the approximate internal charge deposition as the fraction of electrons deposited as a function of penetration depth scaled by the CSDA range determined by the predictive formula for N_V^{pre} through convolution of a universal normalized deposition curve.

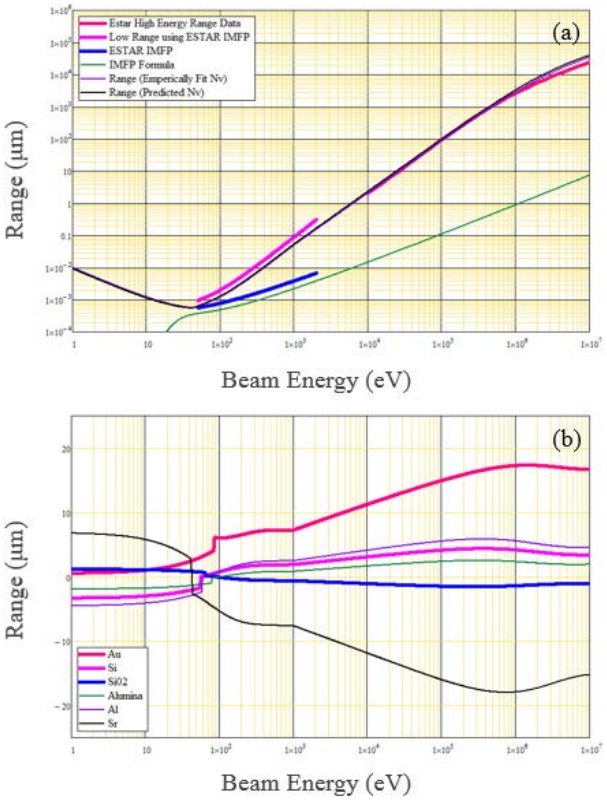

Figure 1. (a) Strontium range calculated using both empirical N_V^{eff} and predicted N_V^{pre} values as compared to ESTAR range data. (b) Percent differences between ranges calculated with empirical N_V^{eff} and predicted N_V^{pre} values, versus incident energy for Al, Au, Si, Sr, Al_2O_3 and SiO_2.

6. REFERENCES

1. National Institute of Standards and Technology, 2010, "ESTAR, Stopping Power and Range Tables for Electrons," (http://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html).
2. National Institute of Standards and Technology, 2010, "NIST Electron Inelastic-Mean-Free-Path Database: Version 1.1," (http://www.nist.gov/data/nist71.htm).
3. Wilson, G., & Dennison, J.R. (2010). Approximation of range in materials as a function of incident electron energy, *IEEE Trans. on Plasma Sci.*, **40**(2), 305-310.
4. T. Quist, B. Moore, G. Wilson and JR Dennison, Electron Penetration Ranges as a Function of Effective Number of Valence Electrons, Utah State University Student Showcase, Logan, UT, April 2013.
5. Starley, A., Phillipps, L., Wilson, G., Dennison, J.R., Predictive Formula for Electron Range over a Large Span of Energies, Am. Phys. Soc. Four Corners Meeting, Mesa, AZ, 2015.